

1,2-Cyclohexanedicarboxylic acid, 2-methylpent-3-yl nonyl ester

Inchi:	InChI=1S/C23H42O4/c1-5-7-8-9-10-11-14-17-26-22(24)19-15-12-13-16-20(19)23(25)27-
InchiKey:	LQMSDKIOQPKZRS-UHFFFAOYSA-N
Formula:	C23H42O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-313.20	kJ/mol	Joback Method
hf	-984.23	kJ/mol	Joback Method
hfus	46.76	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.064		Crippen Method
mvol	338.950	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	892.22	K	Joback Method
tc	1095.57	K	Joback Method
tf	466.43	K	Joback Method
vc	1.292	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.49	J/molxK	892.22	Joback Method
cpg	1176.20	J/molxK	926.11	Joback Method
cpg	1194.34	J/molxK	960.00	Joback Method
cpg	1210.94	J/molxK	993.90	Joback Method
cpg	1226.04	J/molxK	1027.79	Joback Method
cpg	1239.65	J/molxK	1061.68	Joback Method
cpg	1251.81	J/molxK	1095.57	Joback Method
dvisc	0.0009832	Paxs	466.43	Joback Method

dvisc	0.0004013	Paxs	537.39	Joback Method
dvisc	0.0002019	Paxs	608.36	Joback Method
dvisc	0.0001173	Paxs	679.33	Joback Method
dvisc	0.0000755	Paxs	750.29	Joback Method
dvisc	0.0000524	Paxs	821.26	Joback Method
dvisc	0.0000386	Paxs	892.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339446&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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